Substitute Form PTO-1449 (Modified) — U.S. Department of Commerce, Patent and Trademark Office

Information Disclosure Statement by Applicant
(Use several sheets if necessary)

(37 CFR §1.98(b))

Attorney's Docket No.	Application No.
06618-607002	10/010,725
Applicant: Wely B. Floriano, Nagarajan Vaidehi, William A. Goddard, III	
Filing Date: November 30, 2001	Group Art Unit: ~~1645~~ 1631

U.S. Patent Documents

Examiner Initial	Desig. ID	Patent Number	Issue Date	Patentee	Class	Subclass	Filing Date If Appropriate
CDL	AA	5,680,319	10/21/97	Rose et al.	364	496	
	AB	5,705,335	1/6/98	Hendry	435	6	
	AC	5,873,052	2/16/99	Sharaf	702	20	
	AD	5,854,992	12/29/98	Shakhnovich et al.	702	27	
	AE	5,940,307	8/17/99	Fischbarg et al.	364	496	

Foreign Patent Documents or Published Foreign Patent Applications

Examiner Initial	Desig. ID	Document Number	Publication Date	Country or Patent Office	Class	Subclass	Translation Yes	Translation No
	AF							

Other Documents (include Author, Title, Date, and Place of Publication)

Examiner Initial	Desig. ID	Document
CDL	AG	D'Aquino, J. et al., "The Magnitude of the Backbone Conformational Entropy Change in Protein Folding," Proteins: Structure, Function and Genetics (1996) 25:143-156
	AH	Buck, L. et al., "A Novel Multigene Family May Encode Odorant Receptors: A Molecular Basis for Odor Recognition," Cell (1991) 65:175-187
	AI	Burkhard, P. et al., "An Example of a Protein Ligand Found by Database Mining: Description of the Docking Method and Its Verification by a 2.3 Å X-ray Structure of a Thrombin-Ligand Complex," J. Mol. Biol. (1998) 277:449-466
	AJ	Connolly, M.L., "Solvent-Accessible Surfaces of Proteins and nucleic Acids," Science (1983) 221(4612):709-713
	AK	Ding, H. Q. et al., "Atomic Level Simulations on a Million Particles: The Cell Multipole Method for Coulomb and London Nonbond Interactions", J. Chem. Phys. (1992) 97(6):4309-4315
	AL	Datta, D. et al, "Mechanism for Antibody Catalysis of the Oxidation of Water by Singlet Dioxygen" PNAS (2002) 99(5):2636-2641
	AM	Ding, H.Q. et al. "The Reduced Cell Multipole Method for Coulomb Interactions in Periodic Systems with Million-Atom Unit Cells", Chem. Phys. Lett. (1992) 196 (1,2):6-10
	AN	Dombi, G. et al., "Analysis of Protein Transmembrane Helical Regions by a Neural Network", Protein Science (1994) 3:557-566
	AO	Donnelly, D. "Modeling alpha-helical Transmembrane Domains", Biochem. Society Transactions (1993) 21:36-39
	AP	Ewing, T.A. et al., "Critical Evaluation of Search Algorithms for Automated Molecular Docking and Database Screening", J. Comput. Chem. (1997) 18:1175-1189
	AQ	Floriano, W. B. et al., "Molecular mechanisms underlying differential odor responses of a mouse olfactory receptor", PNAS (2002) 97(20):10712-10716
	AR	Gasteiger, J. et al., "Iterative Partial Equalization of Orbital Electronegativity – a Rapid Access to Atomic Charges", Tetrahedron (1980) 36:3219-3288

Examiner Signature	Date Considered
	9/14/04

EXAMINER: Initials citation considered. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.

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CDR	AS	Ghosh , A. et al., "Generalized born model based on a surface integral formulation", J. Phys. Chem. (1998) 102:10983-10990
	AT	Guner, O., Pharmacophore – Perception, Development and Use in Drug Design (2000) 1 – 12
	AU	Huang, E. et al., "*Ab Initio* Fold Prediction of Small Helical Proteins Using Distance Geometry and Knowledge-Based Scoring Functions", Journal of Molecular Biology (1999) 290:267-281
	AV	Jain, A., et al., "A fast recursive algorithm for molecular-dynamics simulation", J. Comp. Phys. (1993) 106:258-268
	AW	Juretic, D. et al., "Conformational Preference Functions for Predicting Helices in Membrane Proteins", Biopolymers (1993) 33:255-273
	AX	Kiyama, R. et al., "Homology Modeling of Gelatinase Catalytic Domains and Docking Simulations of Novel Sulfonamide Inhibitors" Journal of Medicinal Chemistry (1999) 42:1723-1738
	AY	Krautwurst, D. et al., "Identification of Ligands for Olfactory Receptors by Functional Expression of a Receptor Library", Cell (1998) 95:917-926
	AZ	Kuntz, I. et al., "A Geometric Approach to Macromolecule-Ligand Interactions," J. Mol. Biol. (1982) 161:269-288
	AAA	Lim, K. et al., "Molecular Dynamics for Very Large Systems on Massively Parallel Computers: The MPSim Program", J. Comput. Chem. (1997) 18:501-521
	ABB	Malnic, B. et al., "Combinatorial Receptor Codes for Odors", Cell (1999) 96: 713-723
	ACC	Mathiowetz, A.M. et al., "Protein Simulations using Techniques Suitable for Very Large Systems: the Cell Multipole Method for Nonbond Interactions and the Newton-Euler Inverse Mass Operator Method for Internal Coordinate Dynamics", Proteins: Structure, Function, and Genetics (1994) 20:227-247
	ADD	Mayo, S. L. et al. "DREIDING - a generic force field for molecular simulations", J. Phys. Chem. (1990) 94:8897-8909
	AEE	McCammon, J. and Harvey, S.C., Dynamics of Proteins and Nucleic Acids (1987) 51- 84
	AFF	McMartin, C. et al., "QXP: Powerful, Rapid Computer Algorithms for Structure-Based Drug Design", (1997) 11:333-344
	AGG	Mombaerts, P., "Seven-Transmembrane Proteins as Odorant and Chemosensory Receptors", Science (1999) 286:707-711
	AHH	Morris, G.M. et al., "Automated Docking Using a Lamarckian Genetic Algorithm and an Empirical Binding Free Energy Function" J. Comp. Chem. (1998) 19(14):1639-1662
	AII	Palczewski, K., et al., "Crystal Structure of Rhodopsin: A G Protein-Coupled Receptor," Science (2000) 289:739-745
	AJJ	Pilpel, Y. et al. "The variable and conserved interfaces of modeled olfactory receptor proteins" Prot. Sci. (1999) 8:969-977
	AKK	Poincelot, R., et al., "Determination of the Chromophoric Binding Site in Native Bovine Rhodopsin," Biochemistry (1970) 9(8):1809-1816
	ALL	Rappé, A.K. et al., "Charge Equilibration for Molecular Dynamics Simulations", J. Phys. Chem. (1991) 95:3358 –3363
	AMM	Reshetnikova, L. et al., "Crystal Structures of Phenylalanyl-tRNA Synthetase Complexed with Phenylalanine and a Phenylalanyl-adenylate Analogue", J. Mol. Biol. (1999) 287:555-568

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CDL	ANN	Sachdeva, A. et al., "Nasal Mucociliary Clearance & Mucus *p*H in patients with Diabetes Mellitus," Indian J. Med. Res. (1993) 98:265-268
	AOO	Sansom, M. et al., "Modeling Transmembrane Helix Bundles by Restrained MD Simulations", Chapter 14 (pp. 325-347), In Webster, D., Protein Structure Prediction: Methods and Protocols (2000)
	APP	Schertler, G.F.X. , "Structure of rhodopsin", Eye (1998) 12:504-510
	AQQ	Sharma N., et al., "Efficient introduction of aryl bromide functionality into proteins in vivo", FEBS Lett. (2000) 467:37-40
	ARR	Shoichet B.K. et al., "Ligand Solvation in Molecular Docking", Proteins: Structure, Function and Genetics (1999) 34:4-16
	ASS	Schoichet, B.K. et al., "Structure-Based Discovery of Inhibitors of Thymidylate Synthase," Science (1993) 259:1445-1450
	ATT	Singer, M. et al., "Molecular Modeling of Ligand-Receptor Interactions in the OR5 Olfactory Receptor", (1994) Neuroreport 5:1297-1300
	AUU	Singer, M.S., "Analysis of the Molecular Basis for Octanal Interactions in the Expressed Rat 17 Olfactory Receptor," Chem. Senses (2000) 25:155-165
	AVV	Singer, M.S. et al. "Positive Selection Moments Identify Potential Functional Residues in Human Olfactory Receptors", Receptors and Channels (1996) 4:141-147
	AWW	Tannor, D. et al. "Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory", J. Am. Chem. Soc. (1994) 116:11875-11882
	AXX	Uechi et al., "An Automated Structure Prediction System by Lattice Model for Seven-Helix-Type Membrane Proteins", Genome Informatics (1999) 10:239-240
	AYY	Vaidehi, N. et al., "Prediction of Structure and Function of G Protein-Coupled Receptors", PNAS (2002) 99:12622-12627
	AZZ	Vaidehi, N. et al. "Constant Temperature Constrained Molecular Dynamics: The Newton-Euler Inverse Mass Operator Method", J. Phys. Chem. (1996) 100:10508-10517
	AAAA	Vriend, G., "WHAT IF: a molecular modeling and drug design program", J. Mol. Graph. (1990) 8:52-56
	ABBB	Williams, R.L., et al., "Empirical Solvation Models in the Context of Conformational Energy Searches: Application to Bovine Pancreatic Trypsin Inhibitor," Proteins: Structure, Function, and Genetics (1992) 14:110-119
	ACCC	Zou, X., et al., "Inclusion of Solvation in Ligand Binding Free Energy Calculations Using the Generalized-Born Model, " J. Am. Chem. Soc. (1999) 121:8033-8043
	ADDD	Floriano, W.B. et al., "Design of Lead Antagonists for Transcriptional Regulation of Glucocorticoid Responsive Elements," U.S. Provisional Application No. 60/233,294, filed 09/15/00

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